SPECTROCHIMICA ACTA

PART A: MOLECULAR AND BIOMOLECULAR SPECTROSCOPY

LIST OF CONTENTS AND AUTHOR INDEX

VOLUME 51A, 1995

MOLECULAR SPECTROSCOPY

Editors

SIDNEY KETTLE

Norwich, UK

and

JEFFREY STEINFELD

Cambridge, MA, USA

BIOMOLECULAR SPECTROSCOPY

Editors

ARNOLD HOFF

Leiden, The Netherlands

and

JAMES NORRIS

Chigago, IL, USA

ELSEVIER

SPECTROCHIMICA ACTA PART A

MOLECULAR SPECTROSCOPY

EDITORS
Professor Sidney Kettle, *School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, U.K.*
Professor Jeffrey Steinfeld, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.*

ASSOCIATE EDITOR
Professor P. J. Hendra, *Department of Chemistry, University of Southampton, Southampton SO17 1BJ, U.K.*

REVIEWS EDITOR
Professor Michael D. Morris, *Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-1055, U.S.A.*

EDITORIAL ADVISORY BOARD

R. Bacis, *Villeurbanne, France*
J. Broekaert, *Dortmund, Germany*
A. Campion, *Austin, TX*
M. A. Chesters, *Norwich, U.K.*
A. R. H. Cole, *Perth, Australia*
J. A. Coxon, *Halifax, Nova Scotia*
J. S. Francisco, *West Lafayette, IN*
J. E. Griffiths, *Savannah, GA*
P. Griffiths, *Moscow, ID*
H. H. Günthard, *Zurich, Switzerland*
D. Hadži, *Ljubljana, Slovenia*
M. C. Heaven, *Atlanta, GA*
J. Lascombe, *Bordeaux, France*
W. D. Lawrance, *Bedford Park, Australia*
A. C. Legon, *Exeter, U.K.*
A. W. Mantz, *New London, CT*
D. C. McKean, *Edinburgh, U.K.*
J. Mink, *Budapest, Hungary*
C. N. R. Rao, *Bangalore, India*
J. Riveros, *São Paulo, Brazil*
N. Sheppard, *Norwich, U.K.*
W. Slavin, *Ridgefield, CT*
R. E. Sturgeon, *Ottawa, Ontario*
M. Tasumi, *Tokyo, Japan*
V. Vaida, *Boulder, CO*
S. C. Wallace, *Toronto, Ontario*
J. White, *Canberra, Australia*
C. Zhang, *Dalian, P.R.C.*

BIOMOLECULAR SPECTROSCOPY

EDITORS
Professor Arnold J. Hoff, *Huygens Laboratory, Leiden University, 2300 RA Leiden, The Netherlands*
Professor James R. Norris, *Department of Chemistry, University of Chicago, 5735 S. Ellis Avenue, Chicago, IL 60637, U.S.A.*

EDITORIAL ADVISORY BOARD

L. Banci, *Florence, Italy*
S. G. Boxer, *Stanford, CA*
J. Breton, *Gif-sur-Yvette, France*
R. E. Dale, *Madrid, Spain*
C. M. Dobson, *Oxford, U.K.*
J. Fajer, *Upton, NY*
G. Giacometti, *Padua, Italy*
R. Griffin, *Cambridge, MA*
H. J. M. de Groot, *Leiden, The Netherlands*
C. Hilbers, *Nijmegen, The Netherlands*
K. Hodgson, *Stanford, CA*
D. Holten, *St. Louis, MO*
A. R. Holzwarth, *Mühlheim, Germany*
P. J. Hore, *Oxford, U.K.*
R. Kaptein, *Utrecht, The Netherlands*
Y. Koyama, *Nishinomiya, Japan*
Y. Levine, *Utrecht, The Netherlands*
J. Lugtenburg, *Utrecht, The Netherlands*
M. Lutz, *Gif-sur-Yvette, France*
W. Mäntele, *Freiburg, Germany*
D. Marsh, *Göttingen, Germany*
J.-L. Martin, *Palaiseau, France*
J. Miller, *Argonne, IL*
K. Möbius, *Berlin, Germany*
B. Nordén, *Göteborg, Sweden*
W. L. Peticolas, *Eugene, OR*
G. J. Small, *Ames, IA*
M. Stockburger, *Göttingen, Germany*
A. Thomson, *Norwich, U.K.*
W. Zinth, *München, Germany*

Information for Advertisers: Advertising orders and enquiries can be sent to the Advertising Manager, Elsevier Science, Advertising Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands. Tel: +31 20 485 3796; Fax: +31 20 485 3810. *UK:* T.G. Scott & Son, Portland House, 21 Narborough Road, Cosby, Leicestershire LE9 5TA. Tel: +44 116 275 0521; Fax: +44 116 275 0522, attn. Vanessa Bird. *USA, Canada:* Weston Media Associates, Daniel S. Lipner, P.O. Box 1110, Greens Farms, CT 06436-1110, USA. Tel: +1 203 261 2500; Fax: +1 203 261 0101.

One volume *per annum*. Published monthly plus additional issues in July and November.

Annual Institutional Subscription Rates 1995: North, Central and South America, U.S. $1416.00; Rest of World, £950.00. Associated Personal Subscription Rates are available on request for those whose institutions are library subscribers. Sterling prices exclude VAT. Non-VAT registered customers in the European Community will be charged the appropriate VAT in addition to the price listed. Prices include postage and insurance and are subject to change without notice.

Subscription enquiries from customers in North America should be sent to: Elsevier Science Inc., 660 White Plains Road, Tarrytown, NY 10591-5153, U.S.A., and for the remainder of the world to: Elsevier Science Ltd, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, U.K.
Second class postage paid at NEWARK, NJ, and additional mailing offices. **POSTMASTER**: send address corrections to *Spectrochimica Acta Part A*, c/o Elsevier Science Inc., 660 White Plains Road, Tarrytown, NY 10591-5153, U.S.A.

Copyright © 1995 Elsevier Science B.V.

ELSEVIER

SPECTROCHIMICA ACTA
PART A

CONTENTS OF VOLUME 51, 1995

No. 1

MOLECULAR SPECTROSCOPY

Mohamed Mokhtar Mohamed 1 Fourier transform infrared/photoacoustic study of pyridine adsorbed on silica supported copper–molybdenum catalysts

D. Atzei, D. De Filippo, A. Rossi, R. Caminiti and C. Sadun 11 XPS and LAXS study of 1,3-thiazolidine-2-thione and its complexes with Co(II) and Zn(II)

D. Bougeard, J.R. Burie, Nguyen Quy Dao and B. Hennion 21 Lattice dynamical study of an internal charge transfer molecular crystal: 4-nitropyridine *N*-oxide and its deuterated derivative

John A. Timney 33 Energy factored C–O and N–N force constants for the $Ni(CO)_{4-x}(N_2)_x$ series ($x = 0$–4)

Juan Roberto Anacona 39 New rotational transitions in $^{14}N^{32}S$ $(X^2\Pi_{3/2})_{r=}$ 0,1 detected by laser magnetic resonance at 561.3 and 618.4 μm

Norman C. Craig, Steven S. Borick, C. Patrick Collier, Julie S. Humm, Hidong Kim and Lac V. Lee 45 Vibrational spectra and assignments for 3,3,4,4-tetrafluorocyclobutene-d_0, -d_1, and -d_2

M. Salagram, K. Madhukar and V. Jayatyagaraju 65 Optical identification of unusual manganese(V) oxyanion trapped in $KH_3(SeO_3)_2$ crystals

Anju Batra, R. D'Cunha, M.N. Deo, V. Parthasarathy and S.K. Sarkar 71 High resolution FTIR spectral studies of $^{13}CF_3Br$: the degenerate C–F stretch

Sunila Abraham and G. Aruldhas 79 Infrared and polarized Raman spectra of $M(HCOO)_2{\cdot}2(NH_2)_2CO$ [M is Cd, Mn]

B. Kramer, J. Fleischhauer, K.W. Mandelatz und P.H. Laur 89 UV- und MCD-Spektren von cyclischen und acyclischen Sulfiden: Interpretation der Meßergebnisse mit Hilfe semiempirischer Methoden

M. Zamama, A. Burneau and R. Mokhlisse 101 IR study of deuterated dickite–DMSO intercalate: $(Al_2Si_2O_5(OH)_4$–$CH_3SOCH_3)$. Effect of particle size on hydroxyl stretching frequencies

BIOMOLECULAR SPECTROSCOPY

Derek Marsh 111 Sensitivity of the continuous-wave saturation of conventional EPR spectra to slow rotational motion

Donatella Carbonera, Giovanni Giacometti and Giancarlo Agostini 115 FDMR spectroscopy of peridinin–chlorophyll-a protein from *Amphidinium carterae*

Tsunenori Nozawa, Masayuki Kobayashi, Zheng-Yu Wang, Shigeru Itoh, Masayo Iwaki, Mamoru Mimuro and Kimiyuki Satoh 125 Magnetic circular dichroism investigation on chromophores in reaction centers of photosystem I and II of green plant photosynthesis

S. Shochat, P. Gast, A.J. Hoff, G.J. Boender, S. van Leeuwen, W.B.S. van Liemt, E. Vijgenboom, J. Raap, J. Lugtenburg and H.J.M. de Groot 135 ^{13}C MAS NMR evidence for a homogeneously ordered environment of tyrosine M210 in reaction centres of *Rhodobacter sphaeroides*

Will K. Kowalchyk, Kevin L. Davis and Michael D. Morris 145 Surface-enhanced resonance Raman spectroscopy of iron–dopamine complexes

F. Verberckmoes and E.L. Esmans 153 Conformational behaviour of some D-arabino-, D-lyxo- and D-xylofuranosyl pyridine C-nucleosides

No. 2

MOLECULAR SPECTROSCOPY

M.S. El-Shahawi 161 Chromium(III) complexes of naturally occuring ligands

M.S. El-Shahawi and S.A. Barakat 171 Spectral and electrochemical studies of D-tartaric and DL-mandelic acids with different chromium ions

Jinghe Yang, Naixing Wang, Yingjie Wang, Weian Liang, Hongmei Ge and Jie Zhou 177 Study of the absorption spectra of 4f electron transitions of the neodymium and erbium complexes with diphacinone and Triton X-100 and its analytical application

Jinghe Yang, Hongmei Ge, Nianqin Jie, Xuozhen Ren, Naixing Wang and Huabin Zou 185 Study on the co-luminescence system of Tb–Gd–BPMPHD–CTMAB and its analytical application

Jan Baran, Austin J. Barnes and Henryk Ratajczak 197 Polarized infrared and Raman spectra of diglycine nitrate single crystal

D.C. McKean, A.L. McPhail, H.G.M. Edwards, I.R. Lewis, W.F. Murphy, V.S. Mastryukov and J.E. Boggs 215 Infrared and Raman spectra of monochloro- and monobromodisilanes, a scaled ab initio force field, intensities, atomic polar tensors and effective charges for Si_2H_5Cl

Alan G. Osborne, Mustafa T. Ahmet, John R. Miller and Joanne F. Warmsley 237 ^{1}H and ^{13}C NMR spectral and X-ray crystallographic study of 3-methyl-2,4-diphenylquinoline. Sterically hindered phenyl groups and the 'pseudo *peri*-proximity' effect

Yuk Y. Sham and Jeffrey A. Joens 247 Temperature dependent near UV molar absorptivities of several small aldehydes in aqueous solution

William P. Griffith and Tse Yuen Koh 253 Vibrational spectra of 1,2-benzenedithiol, 2-aminothiophenol and 2-aminophenol and their SER spectra

K.M. Singh, R.A. Singh and S.N. Thakur 269 Ground state normal vibrations and force field of ethynylbenzene

Yun-Bao Jiang 275 Twisted intramolecular charge transfer of methyl *p*-dimethylaminobenzoate in aqueous *β*-cyclodextrin solution

Research Note

A.A.M. Belal, A.H. Amrallah and M.T. El-Haty 283 Solvent effect on the charge-transfer absorption bands of furfurylidene malononitriles

BIOMOLECULAR SPECTROSCOPY

Willie A. Bueno and Eduardo G. Sobrinho 287 Hydrogen bonds in the cimetidine molecule

F.J. Ramírez and J.T. López Navarrete 293 Force field and normal coordinate calculations for glutamic acid

A. Pawlukojc, L. Bobrowicz, I. Natkaniec and J. Leciejewicz 303 The IINS spectroscopy of amino acids: L- and DL- valine

No. 3

MOLECULAR SPECTROSCOPY

Ken Ohwada and Ginji Fujisawa 309 Laser Raman spectroscopy of some uranyl trinitrate complexes $MUO_2(NO_3)_3$ (M is Cs, Rb, K, NH_4)

H. Ishida and M.T. Huang 319 Infrared spectral assignments for a semicrystalline thermoplastic polyimide

Xue-Mei Wang and Hong-Yuan Chen 333 Investigation of the β-cyclodextrin-quinine inclusion complex in aqueous solution by spectroscopic study

M.I. Redondo, M.V. García, M.J. González-Tejera and J.A.R. Cheda	341	Spectroscopic study of the phase transitions of copper(II) *n*-alkanoates
Ileana Mincu, Alain Allouche, Michèle Cossu, Jean-Pierre Aycard and Jean Pourcin	349	FT-IR identification, characterization and ab initio vibrational analysis of phosgene, oxalyl chloride and 1,2-dichlorocyclobutene-3,4-dione trapped in argon cryogenic matrices
Ranjan Das, Sivaprasad Mitra and Samaresh Mukherjee	363	Intramolecular proton transfer in the first excited singlet state of 4-methyl-2,6-diformylphenol: effect of non-polar and weakly polar aprotic solvents
E.K. Kemsley and P.S. Belton	371	Simulated emission spectra of samples at non-uniform temperature based on numerical solutions of the general radiative transfer equation
J. Lipiński and H. Chojnacki	381	Solvent effect on the spectroscopic properties of indole — semiempirical quantum chemical study
Asim Kumar Chattopadhyay, Sekhar Basu and S.C. Chakraborty	387	Solvent induced fluorescence of 9-chloro-10,10′-bis (dichloromethyleno)-(9′H)-10,10′-dihydro-9,9′-bianthryl (CDDB): twisted intramolecular charge transfer process
C. Téllez S. and J. Gómez Lara	395	Infrared and Raman spectra (solid state) of uranyl 2,4-pentanedionate: $UO_2(acac)_2$
Franco Cataldo	405	Spectroscopical study on C_{60} and C_{70} fullerene solutions in superacids
Jack Barrett	415	The roles of carbon dioxide and water vapour in warming and cooling the Earth's troposphere
Erkki T. Kolehmainen, Katri P. Laihia, Juha M. I. Hyöthläinen and Reijo T. Kauppinen	419	^{1}H, ^{13}C and ^{17}O NMR spectral study of chlorinated 3,4-dihydroxybenzaldehydes (protocatechualdehydes)
G. Suresh, R. Ratheesh, V.U. Nayar, M. Ichikawa and G. Keresztury	429	IR and polarized Raman spectra of a single crystal $Rb_3H(SeO_4)_2$ in the ferroelastic phase
P. Mirti, L. Appolonia, A. Casoli, R.P. Ferrari, E. Laurenti, A. Amisano Canesi and G. Chiari	437	Spectrochemical and structural studies on a Roman sample of Egyptian blue
O. Zakharieva, Th. Woike and S. Haussuehl	447	Normal coordinate analysis of $[Fe(CN)_5NO]^{2-}$ ion in the ground and metastable state
H. Zine, M.H. Baron and A. Piart-Goypiron	457	Influence of the anion and solvent on the ion-pair stability for $(CH_3)_2CHCH=NH^+(CH)_2\cdots X^-$ iminium salts ($X^- = Cl^-$ or BF^{4-}) vibrational study

Research Notes

E.M. Nour, L.A. Shahada, S.A. Sadeek and S.M. Teleb 471 Spectroscopic studies on the reaction of 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane

R.A. Nyquist and R. Streck 475 Infrared and nuclear magnetic resonance spectra structure correlations for alkyl acrylates and alkyl methacrylates in solution

M.T. El-Haty, A.A.M. Belal and A.H. Amrallah 477 A spectroscopic study of amines with violuric acid interactions

BIOMOLECULAR SPECTROSCOPY

Katrin Kneipp, Yang Wang, Ramachandra R. Dasari and Michael S. Feld 481 Near-infrared surface-enhanced Raman scattering (NIR-SERS) of neurotransmitters in colloidal silver solutions

Medini Kanta Pal and Jimut Kanti Ghosh 489 Spectroscopic probe of the competitive binding of ethidium bromide and neomycin to DNA

No. 4

MOLECULAR SPECTROSCOPY

Review

Carol Korzeniewski and Mark W. Severson 499 Applications of infrared spectroscopy in the study of catalytic reactions and related adsorption phenomena on single crystal electrodes: connections between electrochemical and ultra high vacuum surface science

General Papers

Li Jun, Xia Shuping and Gao Shiyang 519 FT-IR and Raman spectroscopic study of hydrated borates

Patrick F. Corcoran, Jagdish K. Vij and Tatiana S. Perova 533 Dispersive Fourier transform far-infrared spectroscopy of aliphatic ketones

S. Ellahi, R.E. Hester and K.P.J. Williams 549 Waveguide resonance Raman spectroscopy of degraded PVC

R.M.S. Alvarez, E.H. Cutin and C.O. Della Védova 555 Conformational and bond properties of chlorosulfonyl isocyanate, $ClSO_2NCO$

Alessandro Bongini, Daria Giacomini, Mauro Panunzio, Giorgio Suzzi-Valli and Paola Zarantonello 563 Studies on *N*-metallo imines: dependence of chemical shift of the ^{13}C iminic carbon from the nature of the nitrogen substituent

C. Ducouret, E. Petersohn, N. Betz and A. Le Moel 567 Fourier transform infrared analysis of heavy ion grafting of poly(vinylidene fluoride)

A. Kudelski and J. Bukowska	573	Influence of photochemical effects on irreversible loss of "active sites" on SERS active silver electrode
Ming Fat Choi and Peter Hawkins	579	The contact charge transfer absorption spectrum of dimethylsulphoxide with oxygen
Lisa George, K. Sankaran, K.S. Viswanathan and C.K. Mathews	587	A matrix-isolation infrared study of the adducts of triethyl phosphate with CCl_4, $CHCl_3$ and CH_2Cl_2
Yuying Chen, Daniel H. Christensen, Ole Faurskov Nielsen, Jens Hyldtoft and Claus J.H. Jacobsen	595	NIR-FT-Raman studies of square-planar palladium(II) and platinum(II) complexes
Jean Jacques Aaron, Mounir Maafi, Cyril Párkányi and Christian Boniface	603	Quantitative treatment of the solvent effects on the electronic absorption and fluorescence spectra of acridines and phenazines. The ground and first excited singlet-state dipole moments
M. Nishio, P. Paillous, M. Khlifi, P. Burston and F. Raulin	617	Infrared spectra of gaseous ethanenitrile in the 3500–250 cm^{-1} region: absolute band intensity and implications for the atmosphere of Titan
Janina R. Heldt, Józef Heldt and Krzysztof Aleksandrzak	623	Luminescence studies of biochromophoric 9-acet-oxyanthracene derivative
Arzu Topacli and Sevim Akyüz	633	4,4′-Bipyridyl: vibrational assignments and force field
Nguyen-Van-Thanh, A. Jean-Louis and C. Brodbeck	643	Infrared band strengths of B_2H_6 from 2400 to 2800 cm^{-1} at room temperature
Wagner B. De Almeida	653	Molecular structure and internal motion in the $(Co_2)_3 \cdot \cdot \cdot$ HCN tetramer
B.P. Maurya, Alex Punnoose, Mohd Umar and R.J. Singh	661	EPR study of Cu^{2+} ion doped in potassium oxalate monoperhydrate single crystal
S.A. Brandán, A. Ben Altabef and E.L. Varetti	669	Vibrational and electronic spectra of vanadyl nitrate, $VO(NO_3)_3$
D.B. Soria and P.J. Aymonino	677	Infrared spectra of pentacyanonitrosylmanganate(3 –) in $K_3[M(CN)_6]$ (M is Fe, Co) matrices
A.M. Coates, D.C. McKean, C. Starcke and W. Thiel	685	Experimental and theoretical infrared intensities of the fundamental bands of zinc, cadmium and mercury dimethyls; electro-optical parameters, atomic polar tensors and effective atomic charges

Beate K. Ehrhardt and Martin Ystenes	699	Ab initio calculation of geometry and vibrational frequencies of the isovalence-electronic tetrahedral species XCl_4^e and YBr_4^e (X is K, Ca, Ga–Kr; Y is Ne–Ca, Ga–Kr)
Xiande Ding and Guozhen Wu	709	The critical Raman intensity behavior of the nitrate ν_1 mode and its thermodynamic interpretation for the phase transitions of crystalline NH_4NO_3
Si-Hai Chen and Xin-Min Ren	717	SERS studies of methylviologen on silver sol and the effect of halide ions
Short Notes		
B. Singh and Preeti Sahai	727	Molecular structure of terbium(III) complexes —effect of anions on coordination number
N. Tsukahara, H. Yamaguchi, M. Higashi, K. Fujimori and T. Takei	729	Electronic spectra and anomalous fluorescence spectra of 7-isopropylazuleno[1,2-*c*]pyridine and 8-isopropylazuleno[1,2*c*]pyridine
K. Chandrasekharan and V.S. Murty	731	ESR study of Ag^{2+} in $CsNO_3$
Pushkin M. Qureshi and S. Muzaffar Ali Andrabi	733	Charge transfer bands of polynitroaromatics–diphenylamine systems
R. Murugan and S. Mohan	735	Vibrational spectra and normal coordinate analysis of *N*,*N*-dimethylpropionamide
	737	Book Reviews

No. 5

MOLECULAR SPECTROSCOPY

B. Galabov, T. Dudev and S. Ilieva	739	Effective bond charges from experimental IR intensities
H.D. Lutz, K. Beckenkamp and St. Peter	755	Laurionite-type M(OH)X (M is Ba, Pb; X is Cl, Br, I) and Sr(OH)I. An IR and Raman spectroscopic study
C.R. Pulham, A.J. Downs, M.J. Goode and I.M. Mills	769	The vibrational spectra of natural and perdeuterated monochlorogallane, $H_2Ga(\mu\text{-}Cl)_2GaH_2$, and an empirical harmonic potential function
E. Suzuki and F. Watari	779	Matrix IR spectra and normal coordinate analysis for sulfine and sulfine-d_2
N.L. Campbell, C.J. Gillis, D. Klapstein, W.M. Nau, W.J. Balfour and S.G. Fougère	787	Vibrational spectra and conformational behaviour of carbonyl isothiocyanates X–CO–NCS, X is F, Cl, Br, MeO, EtO, and acetyl isothiocyanate CH_3–CO–NCS

K. Burgher, Zs. Nemes-Vetéssy, Gy. Vankó, Z. Homonnay, A. Vértes, I. Dékány and M. Szekeres	799	Mössbauer study of a rigid organic microemulsion used as carrier for fixing a methanolic solution of ascorbic acid complexes of iron
E. Faulques, A. Leblanc, P. Molinié, M. Decoster, F. Conan, J.E. Guerchais and J. Sala-Pala	805	Determination of charge transfer in molybdenum complexes of 7,7,8,8-tetracyano-*p*-quinodimethane with vibrational spectroscopy
R.C.M.U. Araújo, J.B.P. da Silva and M.N. Ramos	821	An ab initio study of hydrogen complexes of the X–H · · · π type between acetylene and HF or HCl
M.K. Shukla and P.C. Mishra	831	Electronic spectra, structure and photoisomerization of urocanic acid
J. Sitkowski, L. Stefaniak, L. Nicol, M.L. Martin, G.J. Martin and G.A. Webb	839	Complete assignments of the ^{1}H, ^{13}C and ^{15}N NMR spectra of caffeine
V.B. Pivovarov, S.G. Stepanian, I.D. Reva, G.G. Sheina and Yu.P. Blagoi	843	Infrared spectra and the structure of 1-methyladenine in an argon matrix and solutions
J. Dunkers and H. Ishida	855	Vibrational assignments of *N,N*-bis(3,5-dimethyl-2-hydroxybenzyl)methylamine in the fingerprint region
J. Hanuza and M. Andruszkiewicz	869	Phonon properties and normal coordinate analysis of gallium–oxygen core in $BaLaGa_3O_7$ crystal
S. Lenaerts, J. Roggen and G. Maes	883	FT-IR characterization of tin dioxide gas sensor materials under working conditions
N. Velasco-García, R. Pereiro-García and M.E. Diaz-García	895	Analytical mechanistic aspects of the room temperature phosphorescence of Erythrosine B adsorbed on solid supports as oxygen sensing phases
Research Note		
A. Schulz and Th.M. Klapötke	905	Vibrational frequencies of the isoelectronic tetrahedral species GeF_4 and AsF_4^+. Comparison of experimental data with results from ab initio and density functional theory
Short Note		
M.S. Navati, G.B. Kalkoti, P.R. Jeergal, M.K. Aralakkanavar and M.A. Shashidhar	909	$\Pi^* \leftarrow \Pi$ system in the electronic absorption spectra of some disubstituted phenols

BIOMOLECULAR SPECTROSCOPY

Letter

J.P. Cornard, L. Vrielynck, J.C. Merlin and J.C. Wallet 913 Structural and vibrational study of 3-hydroxyflavone and 3-methoxyflavone

General Papers

P. Tarakeshwar and S. Manogaran 925 Vibrational frequencies of cysteine and serine zwitterions — an ab initio assignment

P. Carmona, M. Molina and A. Lasagabaster 929 Structural study of human growth hormone-releasing factor fragment (1–29) by vibrational spectroscopy.

939 Book reviews

No. 6

MOLECULAR SPECTROSCOPY

I. Kanesaka and K. Oda 941 Infrared study on T β-radiolysis in the $CaSO_4 \cdot 0.5H_2O$–T_2O system

J.E. Eldridge, C.C. Homes, J.M. Williams, A.M. Kini and H.H. Wang 947 The assignment of the normal modes of the BEDT-TTF electron-donor molecule using the infrared and Raman spectra of several isotopic analogs

K. Tavladorakis and J.E. Parkin 961 A normal coordinate analysis of the planar vibrations of s-trifluorobenzene

V. Iliev and V. Alexiev 969 EPR, ^1H, ^{31}P ENDOR, and IR study of Cu(II) and Ni(II) (*O*,*O*-dimethyldithiophosphate) (*N*,*N*-dimethyldithiocarbamate) complexes

S.E. Jayaraj and V. Ramakrishnan 979 Surface-enhanced Raman scattering of 1,5-dihydroxyanthraquinone in silver sol

J. Georges 985 Deviations from Beer's law due to dimerization equilibria: theoretical comparison of absorbance, fluorescence and thermal lens measurements

A.A. El-Azhary 995 Vibrational analysis of the spectra of 1,3,4-oxadiazole and 1,3,4-thiadiazole

M.A. Czarnecki, M. Czarnecka, Y. Liu, Y. Ozaki, M. Suzuki and M. Iwahishi 1005 FT-NIR study of dissociation of decan-1-ol in the liquid phase — I

M. Ystenes, N. Westberg and B.K. Ehrhardt 1017 Ab initio quantum mechanical vibrational analysis of the dimeric A_2X_6 molecules (A is Al, Ga; X is Cl, Br, I)

Jian Dong, Zhihao Sheng and Gi Xue 1031 Near infrared excited surface enhanced Raman scattering from adsorbed layer on nickel by doping with silver

N. Ghoneim and P. Suppan 1043 Solvatochromic shifts of non-dipolar molecules in polar solvents

B.Kr. Manna, S.Ch. Bera and K.K. Rohatgi-Mukherjee 1051 Effect of solvent and pH on the spectral characteristics of *meso*-tetrakis(*p*-hydroxyphenyl) porphyrin in dimethylformamide and dimethylformamide + water mixed solvents

J. Dunkers and H. Ishida 1061 Vibrational assignments of 3-alkyl-2,4-dihydro-6-methyl-2H-1,3-benzoxazines in the fingerprint region

P. Geissler, T.M. Klapötke and H.-J. Kroth 1075 ^{14}N NMR spectra of covalent halogen and arsenic azides: XN_3 (X is Cl, Br, I), $(CH_3)_nAs(N_3)_{3-n}$ ($n = 0, 1, 2$) and $[As(N_3)_4]^+$

D. Banerjee and S. Bagchi 1079 Solvent effect on the spectroscopic properties of ketocyanine dyes: a study of complexation in the ground state

Short Note

B.A. Uzoukwu 1081 Spectrophotometric studies on 4-acyl derivatives of 1-phenyl-3-methylpyrazolone-5 in various solvents

1083 Book Reviews

BIOMOLECULAR SPECTROSCOPY

Jun Hu, Rong Sheng Sheng, Zhi San Xu and Yun'e Zeng 1087 Surface enhanced Raman spectroscopy of lysozyme

Letters

D. Marsh L1 Paramagnetic relaxation enhancement in CW saturation EPR experiments with nuclear relaxation

R. Sjoback, J. Nygren and M. Kubista L7 Absorption and fluorescence properties of fluorescein

A.B. Sigalov L23 Ultraviolet absorption spectroscopic behaviour of oligodeoxynucleotide–cation complexes

No. 7

Special Issue: **High Resolution Fourier Transform Spectrometry in France**

Guest Editors: Roger Bacis and Jean Marie Flaud

P. Connes 1097 Fourier transform spectrometry at Laboratoire Amié Cotton 1964–1974

P.A. Maillard	1105	Recent results in astronomical Fourier transform spectroscopy
P.A. Martin and G. Guelachvili	1117	Modulation and selective detection of transient species in high resolution FTS
A. Valentin	1127	Fourier spectroscopy with a very long optical path length
C. Camy-Peyret	1143	Balloon-borne infrared Fourier transform spectroscopy for measurements of atmospheric trace species
J.J. Plateaux, A. Barbe and A. Delahaigue	1153	Reims high resolution Fourier transform spectro-meter. Data reduction for ozone
P. Luc	1171	High resolution Fourier transform spectrometry in emission and absorption in the visible and UV ranges
J. Vergès, C. Amiot, R. Bacis and A.J. Ross	1191	Laser induced fluorescence and high resolution Fourier transform spectrometry
J.M. Flaud, A. Perrin and C. Camy-Peyret	1217	Fourier transform spectroscopy of asymmetric top molecules
B. Bobin and J. Moret-Bailly	1231	Fourier transform spectroscopy and the vibration–rotation spectra of spherical top molecules
R. Le Doucen and C. Boulet	1239	Lineshape studies by Fourier transform spectrometry in France

No. 8

MOLECULAR SPECTROSCOPY

W.B. Collier and T.D. Klots	1255	Heteroatom derivatives of indene. Part 1. Vibrational frequencies and a refined scaled overlay of the AM1 force field of indole, benzofuran benzothiophene, benzoxazole and benzothiazole
T.D. Klots and W.B. Collier	1273	Heteroatom derivatives of indene. Part 2. Vibrational spectra of benzothiophene and benzothiazole
T.D. Klots and W.B. Collier	1291	Heteroatom derivatives of indene. Part 3. Vibrational spectra of benzoxazole, benzofuran, and indole
B.P. Maurya, A. Punnoose and R.J. Singh	1317	Electron paramagnetic resonance and superposition model investigations of Mn^{2+} ion doped in sodium formate single crystal
L. Seguin, M. Figlarz, R. Cavagnat and J.-C. Lassègues	1323	Infrared and Raman spectra of MoO_3 molybdenum trioxides and $MoO_3 \cdot xH_2O$ molybdenum trioxide hydrates

A. Mortensen and O.F. Nielsen	1345	Vibrational spectra in the carbonyl stretching region of isotopomers of formamide in the gaseous and liquid states
S.M. Quadri and H.F. Shurvell	1355	An infrared spectroscopic study of complex formation between *meta*-cresol and propionitrile
A.F. Bell, L. Hecht and L.D. Barron	1367	Vibrational Raman optical activity of ketose monosaccharides
Hong-Wen Gao	1379	Use of β-correction spectrophotometry to improve the determination of copper solution with erio-chrome black T
Research Note		
L.F. Vieira Ferreira, J.C. Netto-Ferreira and Sílvia M.B. Costa	1385	Time-resolved absorption and emission spectra of triplet state β-phenylpropiophenone adsorbed on silicalite
Comments		
R.K. Harris, M.M. Sünnetçioglu and R.D. Fischer	1389	Correction and comment on "Variable-temperature ^{13}C solid-state NMR spectra: mobility of trimethyltin groups in coordination polymers of the type $[(Me_3Sn)_4M(CN)_6]_x$ (M = Fe, Os, Ru)"
J. Houghton	1391	Comment on "The roles of carbon dioxide and water vapour in warming and cooling the Earth's troposphere"
K.P. Shine	1393	Comment on "The roles of carbon dioxide and water vapour in warming and cooling the Earth's troposphere"
Reply		
J. Barrett	1395	Reply to comments by Sir John Houghton and Keith P. Shine on "The roles of carbon dioxide and water vapour in warming and cooling the Earth's troposphere"

BIOMOLECULAR SPECTROSCOPY

R.A. Shaw, E. Kollát, M. Hollósi and H.H. Mantsch	1399	Hydrogen bonding and isomerization in thioamide peptide derivatives
Review		
R.A. Dluhy, S.M. Stephens, S. Widayati and A.D. Williams	1413	Vibrational spectroscopy of biophysical monolayers. Applications of IR and Raman spectroscopy to biomembrane model systems at interfaces
	1449	Book Reviews
	1453	Errata

1457 Editorial Announcement — Sir Harold Thompson Memorial Award

No. 9

MOLECULAR SPECTROSCOPY

S. Kumar, R. Giri, S.C. Mishra and M.K. Machwe 1459 Photophysical characteristics of the laser dye 7-dimethylamino cyclopenta[c]coumarin

K. Tavladorakis and J.E. Parkin 1469 Rotational analysis of the $\nu_{15}(a_2'')$ and $\nu_{16}(a_2'')$ parallel bands of the mid-infrared spectrum of *s*-tri-fluorobenzene

P.R. Olivato, D.S. Ribeiro, R. Rittner, Y. Hase, D. del Pra and G. Bombieri 1479 Stereochemical and electronic interaction studies of α-heterosubstituted acetone oximes

Liu Shaopu and Liu Zhongfang 1497 Studies on the resonant luminescence spectra of rhodamine dyes and their ion-association complexes

M. Ystenes and N. Westberg 1501 Ab initio quantum mechanical vibrational analysis of the dimeric molecules Mg_2F_4, Mg_2Cl_4 and Mg_2Br_4

R. Ratheesh, G. Suresh, M.J. Bushiri and V.U. Nayar 1509 Infrared and polarized Raman spectra of $Cu(HSeO_3)_2 \cdot H_2O$ single crystal

M.L.A. Temperini, M.R. dos Santos and V.R. Paoli Monteiro 1517 Spectroscopic study of the isomerization of *Z*- to *E*-pyridine-2-formyl thiosemicarbazone

M.M. Mohamed and G.M.S. El Shafei 1525 Treatment and halogenation on low molybdenum silica: diffuse reflectance IR Fourier transform study (DRIFTS)

1533 Book Reviews

1537 Announcement — VIIth International Symposisium on Luminescence Spectrometry in Biomedical Analysis

1539 Corrigendum

BIOMOLECULAR SPECTROSCOPY

K.V. Lappalainen, E.T. Kolehmainen and D. Šaman 1543 Interaction of anisole with 3α-hydroxy-5β-cholan-24-oic acid macrolides. Part 1. Comparative ^{1}H NMR spectral investigation

J.R. Heldt, J. Heldt, M. Stoń and H.A. Diehl 1549 Photophysical properties of 4-alkyl- and 7-alkoxycoumarin derivatives. Absorption and emission spectra, fluorescence quantum yield and decay time

S. Schmidt, T. Arlt, P. Hamm, H. Huber, T. Nägele, J. Wachtveitl, W. Zinth, M. Meyer and H. Scheer	1565	Primary electron-transfer dynamics in modified bacterial reaction centers containing pheophytin-a instead of bacteriopheophytin-a
Weizhong Ke and Jianzhong Wu	L25	Comparison of several methods of fluorescence quenching in protein molecules

No. 10

MOLECULAR SPECTROSCOPY

Review

M. Fehér and P.A. Martin	1579	Tunable diode laser monitoring of atmospheric trace gas constituents

General Papers

I. Wolfs and H.O. Desseyn	1601	Hydrogen bond patterns in solid state carboxylic acids. Vibrational study of the hydrogen bond patterns in oxamic, malonamic and succinamic acid
S.H.J. De Beukeleer and H.O. Desseyn	1617	The spectroscopic study of cationic complexes of dithiomalonamide with Ni(II), Pd(II) and Pt(II)
K. Palm	1635	Rot-step attenuated total reflection spectroscopy on oriented poly(vinylidene fluoride)
L. Bistričić, G. Baranović and K. Mlinarić-Majerski	1643	A vibrational assignment of adamantane and some of its isotopomers. Empirical versus scaled semiempirical force field
Jian Wan and Chang-Guo Zhan	1665	Maximum bond order hybrid orbital calculations of the P=S stretching frequencies for organophosphorus compounds
D. Dumont and D. Bougeard	1671	Molecular-dynamical calculations of the vibrational spectra of hydrocarbons adsorbed in silicalite
Jianfang Wang and D.F.R. Gilson	1683	Variable-temperature and variable-pressure vibrational spectroscopic studies of solid tropolone
R.M. Linares, A. González, J.H. Ayala, A.M. Afonso and V. González	1691	Protolytic equilibria of indole and several indolecarboxylic acids in micellar media
A. Bangher, R.G. Guy, Y. Pichot, J.M. Sillence, C.J. Steel, F.J. Swinbourne and K. Tamiatti	1703	Pseudohalogen chemistry. Part 12. NMR and IR studies of substituent effects in 4-substituted thiocyanatobenzenes
N. Butt, R.G. Guy and F.J. Swinbourne	1715	Pseudohalogen chemistry. Part 13. NMR and IR studies of substituent effects in 3- and 3,5-substituted thiocyanatobenzenes
A.A. Stolov, A.I. Morozov and A.B. Remizov	1725	Temperature and solvent effects on the infrared *e*-type bands of methyl iodide: orientational diffusion and free rotation

Xiaolin Sun, Min Zin and Zhe Li	1739	Spectroscopic studies on molecular association: Structures of some *o*-hydroxylbenzenesulfonan-ilides and determination of acidity constants
M.M. Habeeb, E.A. Hamed, A.K. Shehata, F. El-Zahraa M. El-Hegazy	1747	Studies on hydrogen bonded complexes. Proton transfer equilibria and thermodynamic parameters of hydrogen bonded complexes in 2,4-dinitro-1-naphthol–amine systems
M. Santo, J.D. Anunziata, R. Cattana and J.J. Silber	1749	Solvatochromic studies in quinoline and cyanoquinoline. Preferential solvation in alcohol–cyclohexane binary mixtures

BIOMOLECULAR SPECTROSCOPY

S.L. Winder, R.W. Broadhurst and P.J. Hore	1753	Photo-CIDNP of amino acids and proteins: effects of competition for flavin triplets
W. Ziegler and A. Blume	1763	Acyl chain conformational ordering of individual components in liquid-crystalline bilayers of mixtures of phosphatidylcholines and phosphatidic acids. A comparative FTIR and ^{2}H NMR study

No. 11

MOLECULAR SPECTROSCOPY

Review

S.M. Angel, M. Carrabba and T.F. Cooney	1779	The utilization of diode lasers for Raman spectroscopy
G. Pfister-Guillouzo, F. Gracian, J.A. Paez, C.G. Gómez and J. Elguero	1801	Study of 1-hydroxybenzotriazole/benzotriazole *N*-oxide tautomerism in the gas phase by photoelectron spectroscopy
D. Prusinowska, L. Lapinski, M.J. Nowak and L. Adamowicz	1809	Tautomerism, phototautomerism and infrared spectra of matrix-isolated 2-quinolinethione
Feng Wang and E.I. von Nagy-Felsobuki	1827	Ab initio rovibrational states of the D_{3h} and C_{2v} isotopomers of Li_3^+
C. Martín, I. Martín, V. Rives, S. Damyanova and A. Spojakina	1837	Characterization and Fourier transform infrared spectroscopic study of surface acidity in $NiMo/TiO_2–Al_2O_3$ catalysts
L.M. Nxumalo and T.A. Ford	1847	Ab initio calculations of the structural, energetic and vibrational properties of some hydrogen bonded and van der Waals dimers. Part 2. Sulphur dioxide
E. Lamcharfi, G. Kunesch, C. Meyer and B. Robert	1861	Investigation of cyclodextrin inclusion compounds using FT-IR and Raman spectroscopy
I. Binev, E. Velcheva and I. Juchnovski	1871	On the validity of the constants of ionic substi-tuents. Substituent effects on the cyano stretching frequencies and intensities of *trans*-α-phenyl-β-arylacrylonitriles

J.M.L. Poyato, J.J. Camacho, A.M. Polo and A. Pardo 1879 Radiative transition probabilities for the $B\ ^1\Pi_u \rightarrow X\ ^1\Sigma_g^+$ band system of Na_2 excited by the 4658 Å line of the argon ion laser

N. Pietri, J.P. Aycard, A. Allouche, P. Verlaque and T. Chiavassa 1891 Identification of a predominant keto conformer of malonyl dichloride: An infrared and theoretical study

Hongguang Zhang, Fanchen Liu, Tianjin He and Howen Xin 1903 Time dependent UV-absorption spectra and surface enhanced Raman scattering of pyridine in AgCl sol

Jian-Wei Xie, Jin-Gou Xu and Guo-Zhen Chen 1909 Sensitized room temperature phosphorescence of biacetyl in reversed micelles

A.A. Stolov and A.B. Remizov 1919 Thermodynamic parameters of conformational equilibrium in 1,2-dichloroethane: influence of medium, benzene and compensation effects

Short Notes

A.A. Hassan 1933 Spectroscopic and thermodynamic studies of charge transfer complexes of some aryl-3-aminomethyl-2-mercaptobenzimidazoles with π-acceptors

V.E. Borisenko, N.V. Sokolovskaja, L.A. Kuzina and A. Koll 1935 Dynamic and electrooptical nonequivalency of NH bonds in ortho substituted anilines with intra- and intermolecular hydrogen bonds

BIOMOLECULAR SPECTROSCOPY

M. Engelke, H.-C. Klockmann and H.A. Diehl 1939 Gramicidin effects on the transverse and lateral distribution of pyrene and pyrene derived probes in lipid bilayers

Ying Hu, T. Mizoguchi, Y. Kurimoto and Y. Koyama 1949 Isolation by high-pressure liquid chromatography of cis–trans isomers of β-apo-12′-carotenal and determination of their configurations by ^1H NMR spectroscopy

E. Gaggelli, N. Gaggelli, A. Maccotta, G. Valensin, D. Marini, M.E Di Cocco and M. Delfini 1959 Determination of intramolecular hydrogen bonds in amikacin in water solution by NMR spectroscopy

S. Stoeva, P. Dolashka, B. Bankov, W. Voelter, B. Salvato and N. Genov 1965 Spectroscopic properties of *Callinectes sapidus* hemocyanin subunits

No. 12

Special Issue: **Application of Fourier Transform Raman Spectroscopy — V**

Guest Editor: Patrick Hendra

v Editorial

Instrumental

Research Note

G. Dent 1975 The use of Nujol mulls as FT Raman samples

Papers

J.P. Caudin, A. Beljebbar, G.D. Sockalingum, J.F. Angiboust and M. Manfait	1977	Coupling FT Raman and FT SERS microscopy with TLC plates for in situ identification of chemical compounds
I.R. Lewis, N.W. Daniel, Jr., N.C. Chaffin, P.R. Griffiths and N.W. Tungol	1985	Raman spectroscopic studies of explosive materials: towards a fieldable explosives detector
R. Bennett	2001	Applications of a modulated laser for FT Raman spectroscopy. Part 2. Signal-to-noise enhancement and removal of thermal backgrounds

Inorganics

S.J.A. Pope and Y.D. West	2011	Use of the FT Raman spectrum of Na_2MoO_4 to study sample heating by the laser
C. Ludwig and H.-J. Götze	2019	Fourier transform Raman and infrared spectra and normal coordinate analysis of $(C_6H_5)_3Bi$ and $(C_6D_5)_3Bi$
S.J.A. Pope and Y.D. West	2027	Comparison of the FT Raman spectra of inorganic tetrahedral ions over the temperature range 77 to 473 K

Organic

J.M. Alía, H.G.M. Edwards and J. Moore	2039	Solvation of Ag^+ ions in some nitriles; a Fourier transform Raman spectroscopic study
E.E. Lawson, H.G.M. Edwards and A.F. Johnson	2057	FT Raman spectroscopic study of the wavenumber region 2800–2630 cm^{-1} of selected organic compounds
S.F. Parker	2067	Vibrational spectroscopy of *N*-methylmaleimide

Biological

H.G.M. Edwards and D.W. Farwell	2073	Ivory and simulated ivory artefacts: Fourier transform Raman diagnostics study
A. Beljebbar, G.D. Sockalingum, J.F. Angiboust and M. Manfait	2083	Comparative FT SERS, resonance Raman and SERRS studies of doxurubicin and its complex with DNA
H.G.M. Edwards, N.C. Russell, M.R.D. Seaward and D. Slarke	2091	Lichen biodeterioration under different microclimates: an FT Raman spectroscopy

Polymers

J.K.F. Tait, H.G.M. Edwards, D.W. Farwell and J. Yarwood	2101	Fourier transform Raman spectroscopic examination of two amine-based epoxy resin crosslinking agents

M.V. Pellow-Jarman, P.J. Hendra and M.J.J. Hetem	2107	Poly(butylene terephthalate) polycarbonate transesterification: monitoring its progress with Fourier transform Raman spectroscopy
M. Arruebarrena de Báez, P.J. Hendra and M. Judkins	2117	The Raman spectra of oriented isotactic polypropylene
P.A. Bentley and P.J. Hendra	2125	Polarised FT Raman studies of an ultra-high modulus polyethylene rod
B.H. Stuart and P.S. Thomas	2133	Xylene swelling of polycarbonate studied using Fourier transform Raman spectroscopy
G. Ellis, F. Román, C. Marco, M.A. Gómez and J.G. Fatou	2139	FT Raman study of orientation and crystallization processes in poly(ethylene terephthalate)

SERS and surfaces

R. Ferwerda and J.H. van der Maas	2147	The influence of adsorbed molecules on the framework vibrations of Na-Faujasites studied with FT Raman spectroscopy
Y. Chen, J. Hyldtoft, C.J.H. Jacobsen and O.F. Nielsen	2161	NIR FT Raman spectroscopic studies of η-Al_2O_3 and Mo/η-Al_2O_3 catalysts
K. Kniepp, Y. Wang, R.R. Dasari, M.S. Field, B.D. Gilbert, J. Janni and J.I. Steinfeld	2171	Near-infrared surface-enhanced Raman scattering of trinitrotoluene on colloidal gold and silver
Tse Yuen Koh	2177	SERS of dithiocarbamates and xanthates

Pharmaceuticals

T.M. Hancewicz and C. Petty	2193	Quantitative analysis of vitamin A using Fourier transform Raman spectroscopy

Education

S.B. Abhyankar and S. Subramanian	2199	Raman spectroscopy in undergraduate chemical education
Report		
P.J. Hendra	2205	Teaching Raman spectroscopy at undergraduate level
Letter		
G. Dent	2209	The gap between experienced spectroscopists and part-time users

No. 13

MOLECULAR SPECTROSCOPY

Review		
A.W. Mantz	2211	A review of spectroscopic applications of tunable semiconductor lasers

General Papers

D.C. McKean, H.G.M. Edwards, I.R. Lewis, W.F. Murphy, V.S. Mastryukov and J.E. Boggs	2237	Infrafed and Raman spectra of 1,1-dichlorodisilane species: a scaled ab initio force field, atomic polar tensors, dipole derivatives and atomic charges
M. Fields, R. Devonshire, H.G.M. Edwards and V. Fawcett	2249	Laser-Raman spectroscopic study of the vapour phase equilibria above molten $SnCl_2$
K. Tavladorakis and J.E. Parkin	2267	The perpendicular fundamental bands of the mid-infrared spectrum of s-trifluorobenzene-h_3
K. Tavladorakis and J.E. Parkin	2273	A normal coordinate analysis of the out-of-plane vibrations of s-trifluorobenzene
Sk. Asrof Ali, A. Hassan and M.I.M. Wazeer	2279	NMR study of the anomeric effect and nitrogen inversion in some isoxazolidines
B.S. Panigrahi, S. Peter, K.S. Viswanathan and C.K. Mathews	2289	Fluorescence enhancement of TB^{3+} in Tb–aromatic acid complexes: correlation of synergistic enhancement with the structure of the ligand
K. Choi and D.W. Tedder	2301	Nuclear magnetic resonances of tri-*n*-butyl phosphate-diluent mixtures
T.D. Klots	2307	Vibrational spectra of indene. Part 4. Calibration, assignment, and ideal-gas thermodynamics
W.C. Moreira and R. Aroca	2325	Spectroscopic and gas adsorption properties of thulium bisphthalocyanine Langmuir–Blodgett films
N.I. Nijegorodov and W.S. Downey	2335	The influence of symmetrical substitution on fluorescence parameters and the intersystem crossing rate constant in aromatic molecules
J. Casado, J.T. López Navarrete and F.J. Ramírez	2347	Force field and normal coordinate calculations of the amino acid L-asparagine
C. Vogel-Weill and J. Corset	2357	Spectres infrarouge et Raman de l'acide stéarique et d'une série d'acides gras forme C: modes de squelette, couplage des modes longitudinaux acoustiques (LAM1, LAM3) avec les modes dans le plan de la liaison hydrogène du dimère en dessous de 700 cm^{-1}
M.F. Budyka and N.D. Sokolov	2379	Description of electron donor–acceptor complexes by a simple MO method: comparison of spectral properties of symmetric DAD and asymmetric ADD complexes
S.E. Cabaniss and I.F. McVey	2385	Aqueous infrared carboxylate absorbances: aliphatic monocarboxylates
D.A. Zimmerman, J.L. Koenig and H. Ishida	2397	Infrared spectroscopic analysis of poly(*p*-phenylene sulfide)
V. Pop and D. Dorohoi	2411	A study of the spectra of microparticles in suspension in the liquid state

Short communication

Sheng-Gang Yan, Ai-Li Zhang and Keyan Zhou 2421 The ^1H (Se–H) NMR of aryl selenols; an interesting correlation between the ^1H (Se–H) chemical shift and the Hammett constant

2429 Book reviews

2431 Announcement — Third International Conference on Applications of Magnetic Resonance in Food Sciences

No. 14

MOLECULAR SPECTROSCOPY

Review

Y. Maeda and H. Kitano 2433 The structure of water in polymer systems as revealed by Raman spectroscopy

General Papers

H. Saito, H. Kurabe, E. Suzuki and F. Watari 2447 Matrix IR spectra and normal coordinate analysis for methanesulfenyl chloride and isotopic analogs

S. Parthiban, B.N. Raghunandan and R. Sumathi 2453 Ab initio quantum chemical calculations of geometry and vibrational frequencies of chlorine heptoxide

Su Qingde, Mao Qinglu and Zhao Guiwen 2459 Photoacoustic spectra of $Nd(TFA)_3 \cdot 2H_2O$ and $Nd(HFA)_3 \cdot 2H_2O$

V. Prezhdo, O. Prezhdo and E. Ovsiankina 2465 Synthesis of 2-chloroalkyl-1,4-naphthoquinones and their reactivity in the formation of autocomplexes

S. Arathi Rani, J. Sobhanadri and T.A. Prasada Rao 2473 Determination of the excited state dipole moment of fluorenone using the method of solvatochromism

B.K. Ystenes, M. Ystenes and G. Scholz 2481 Ab initio quantum mechanical vibrational analysis of planar AX_3 molecules (A is Al, Ga, In; X is F, Cl, Br, I)

M. Towrie, P. Matousek, A.W. Parker, W.T. Toner and R.E. Hester 2491 The picosecond transient Raman spectra of S_1 excited oligophenyls, oxazols and stilbene derivatives

Haongguang Zhang, Fanchen Liu, Yujin Wang, Xiuyan Wang, Jian Zuo, Chungi Xu, Tianjin He and Howen Xin 2501 Surface enhanced Raman scattering observation of quinhydrones formation from the reaction of hydroquinone reducing silver bromide sol

J.Y. Zhou, R.H. Li, D.J. Zhou, J.X. Meng and Y.S. Yang 2511 Probing the microstructures of trivalent rare earth compounds with time-resolved two-center cooperative vibronic spectroscopy

L.I. Kozhevina, E.B. Prokopenko, V.I. Rybachenko and E.V. Titov 2517 The influence of the fluorosubstituence on the intensity of C=N valence vibrations in aromatic Schiff bases

A.G. Osborne, R.J. Cremlyn and J.F. Warmsley	2525	Re-examination of the ^{13}C NMR spectrum of xanthene: a revised correlation for the carbocyclic ring $^{3}J_{CH}$ *meta*-coupling constants in fused oxygen het-erocycles
J.L. Rao, V. Padmavathi, K.V. Narasimhulu and Y. Nagaraja Naidu	2531	Electron paramagnetic resonance and optical absorption studies of Cu(II) ions in cadmium malate pentahydrate single crystals
D. Bhattacharjee, A. Ghosh (Purkayastha), T.N. Misra and S.K. Nandy	2539	The non-coincidence effect in polar liquids
A.L. Mattioda and R. Frech	2545	Vibrational modes of hydrazine sulfate and deuterium-substituted single crystals
Y. Hase	2561	Theoretical study of the force field and vibrational assignments of acetamide and deuterated analogues
Ch.P.F. Borges, S. Honda, R.G.S. Berlinck, H. Imasato, P. Berci Filho and M. Tabak	2575	Synthesis, characterization and interaction with ionic micelles of tetraacetylated dipyridamole
Short notes		
J.M.A. Al-Rawi, S.Y. Hanna and A.A. Al-Rhman	2585	Solvent effects on the ^{1}H NMR spectra of α-(2-hydroxy-1-phenyl)-*N*-(4-substituted phenyl nitrones
A.A.M. Belal, M.T. El-Haty, A.A. Ibrahium and A.A. Gabs	2587	Spectral characteristics of some Schiff bases derived from 2-furfuraldehyde
	2591	Book reviews

ELSEVIER

SPECTROCHIMICA ACTA
PART A

AUTHOR INDEX

Aaron, J.J., 603
Abhyankar, S.B., 2199
Abraham, S., 79
Adamowicz, L., 1809
Afonso, A.M., 1691
Agostini, G., 115
Ahmet, M.T., 237
Akyüz, S., 633
Aleksandrzak, K., 623
Alexiev, V., 969
Alía, J.M., 2039
Allouche, A., 349, 1891
Al-Rawi, J.M.A., 2585
Al-Rhman, A.A., 2585
Alvarez, R.M.S., 555
Amiot, C., 1191
Amrallah, A.H., 283, 477
Anacona, J.R., 39
Andrabi, S.M.A., 733
Andruszkiewicz, M., 869
Angel, S.M., 1779
Angiboust, J.F., 1977, 2083
Anunziata, J.D., 1749
Appolonia, L., 437
Aralakkanavar, M.K., 909
Arathi Rani, S., 2473
Araújo, R.C.M.U., 821
Arlt, P., 1565
Aroca, R., 2325
Arruebarrena de Báez, M., 2117
Aruldhas, G., 79
Asrof Ali, Sk., 2279
Atzei, D., 11
Ayala, J.H., 1691
Aycard, J.P., 349, 1891
Aymonino, P.J., 677

Bacis, R., 1191
Bagchi, S., 1079
Balfour, W.J., 787
Banerjee, D., 1079
Bangher, A., 1703
Bankov, B., 1965
Barakat, S.A., 171
Baran, J., 197
Baranović, G., 1643
Barbe, A., 1153
Barnes, A.J., 197
Baron, M.H., 457
Barrett, J., 415, 1395
Barron, L.D., 1367
Basu, S., 387
Batra, A., 71
Beckenkamp, K., 755
Belal, A.A.M., 283, 477, 2587
Beljebbar, A., 1977, 2083
Bell, A.F., 1367
Belton, P.S., 371
Ben Altabef, A., 669
Bennett, R., 2001
Bentley, P.A., 2125
Bera, S.Ch., 1051
Berci Filho, P., 2575
Berlinck, R.G.S., 2575
Betz, N., 567
Bhattacharjee, D., 2539
Binev, I., 1871
Bistričić, L., 1643
Blagoi, Yu.P., 843
Blume, A., 1763
Bobin, B., 1231
Bobrowicz, L., 303
Boender, G.J., 135
Boggs, J.E., 215, 2237
Bombieri, G., 1479
Bongini, A., 563
Boniface, C., 603
Borges, Ch.P.F., 2575
Borick, S.S., 45
Borisenko, V.E., 1935
Bougeard D., 21, 1671
Boulet, C., 1239
Brandán, S.A., 669
Broadhurst, R.W., 1753
Brodbeck, C., 643
Bruston, P., 617
Budyka, M.F., 2379
Bueno, W.A., 287
Bukowska, J., 573
Burgher, K., 799
Burie, J.R., 21
Burneau, A., 101
Bushiri, M.J., 1509
Butt, N., 1715

Cabaniss, S.E., 2385
Camacho, J.J., 1879
Caminiti, R., 11
Campbell, N.L., 787
Camy-Peyret, C., 1143, 1217
Canesi, A.A., 437
Carbonera, D., 115
Carmona, P., 929
Carrabba, M., 1779
Casado, J., 2347
Casoli, A., 437
Caudin, J.P., 1977
Cataldo, F., 405
Cattana, R., 1749
Cavagnat, R., 1323
Chakraborty, S.C., 387
Chandrasekharan, K., 731
Chaffin, N.C., 1985
Chattopadhyay, A.K., 387
Cheda, J.A.R., 341
Chen, Guo-Zhen, 1909
Chen, Si-Hai, 717
Chen, Y., 2161
Chen, Yuying, 595
Chiari, G., 437
Chiavassa, T., 1891
Choi, K., 2301
Choi, Ming Fat, 579
Chojnacki, H., 381
Christensen, D.H., 595
Coates, A.M., 685
Collier, C.P., 45, 1255, 1273, 1291
Conan, F., 805
Connes, P., 1097
Cooney, T.F., 1779
Corcoran, P.F., 533
Cornard, J.P., 913
Corset, J., 2357
Cossu, M., 349
Costa, S.M.B., 1385
Craig, N.C., 45
Cremlyn, R.J., 2525
Cutin, E.H., 555
Czarnecka, M., 1005
Czarnecki, M.A., 1005

da Silva, J.B.P., 821
de Groot, H.J.M., 135
del Pra, D., 1479
dos Santos, M.R., 1517
Damyanova, S., 1837
Daniel Jr., N.W., 1985
Dasari, R.R., 481, 2171
Das, R., 363
Davis, K.L., 145
Dao, Nguyen Quy, 21
D'Cunha, R., 71
De Almeida, W.B., 653
De Beukeleer, S.H.J., 1617
Decoster, M., 805
De Filippo, D., 11
Dékány, I., 799
Delahaigue, A., 1153
Della Védova, C.O., 555
Delfini, M., 1959
Dent, G., 1975, 2209
Deo, M.N., 71
Desseyn, H.O., 1601, 1617
Devonshire, R., 2249
Diaz-García, M.E., 895
Di Cocco, M.E., 1959
Diehl, H.A., 1549, 1939
Ding, Xiande, 709
Dluhy, R.A., 1413
Dolashka, P., 1965
Dong, Jian, 1031
Dorohoi, D., 2441

Downey, W.S., 2335
Downs, A.J., 769
Ducouret, C., 567
Dudev, T., 739
Dumont D., 1671
Dunkers, J., 855, 1061

Edwards, H.G.M., 215, 2039, 2057, 2073, 2091, 2101, 2237, 2249
Ehrhardt, B.K., 699, 1017
El-Azhary, A.A., 995
Eldridge, J.E., 947
Elguero, J., 1801
El-Haty, M.T., 283, 477, 2587
El-Hegazy, M., 1747
Ellahi, S., 549
Ellis, G., 2139
El Shafei, G.M.S., 1525
El-Shahawi, M.S., 161, 171
El-Zahraa, F., 1747
Engelke, M., 1939
Esmans, E.L., 153

Farwell, D.W., 2073, 2101
Fatou, J.G., 2139
Faulques, E., 805
Fawcett, V., 2249
Fehér, M., 1579
Feld, M.S., 481, 2171
Ferrari, R.P., 437
Ferwerda, R., 2147
Fields, M., 2249
Figlarz, M., 1323
Fischer, R.D., 1389
Flaud, J.M., 1217
Fleischhauer,, J., 89
Ford, T.A., 1847
Fougère, S.G., 787
Frech, R., 2545
Fujimori, K., 729
Fujisawa, G., 309

Gabs, A.A., 2587
Gaggelli, E., 1959
Gaggelli, N., 1959
Galabov, B., 739
García, M.V., 341
Gao, Hong-Wen, 1379
Gao, Shiyang, 519
Gast, P., 135
Gaudin, J.P., 1977
Ge, Hongmei, 177, 185
Geissler, P., 1075
Genov, N., 1965
George, L., 587
Georges, J., 985
Ghoneim, N., 1043
Ghosh, J.K., 489
Ghosh (Purkayastha), A., 2539
Giacometti, G., 115
Giacomini, D., 563
Gilbert, B.D., 2171
Gillis, C.J., 787
Gilson, D.F.R., 1683
Giri, R., 1459
Gómez, C.G., 1801
Gómez, Lara, J., 395
Gómez, M.A., 2139
González, A., 1691
González-Terjera, M.J., 341
González, V., 1691
Goode, M.J., 769
Götze, H.-J., 2019
Gracian, F., 1801
Griffiths, P.R., 1985
Griffith, W.P., 253
Guelachvili, G., 1117
Guerchais, J.E., 805
Guy, R.G., 1703, 1715

Habeeb, M.M., 1747
Hamed, E.A., 1747
Hamm, P., 1565
Hancewicz, T.M., 2193
Hanna, S.Y., 2585
Hanuza, J., 869
Harris, R.K., 1389
Hase, Y., 1479, 2561
Hassan, A., 2279
Hassan, A.A., 1933
Haussuehl, S., 447
Hawkins, P., 579
Hecht, L., 1367
He, Tianjin, 1903, 2501
Heldt, J., 623, 1549
Heldt, J.R., 623, 1549
Hendra, P.J., 2107, 2117, 2125, 2205
Hennion, B., 21
Hester, R.E., 549, 2491
Hetem, M.J.J., 2107
Higashi, M., 729
Hoff, A.J., 135
Hollósi, M., 1399
Homes, C.C., 947
Homonnay, Z., 799
Honda, S., 2575
Hong-Yuan, Chen, 333
Hore, P.J., 1753
Houghton, J., 1391
Huang, M.T., 319
Huber, H., 1565
Humm, J.S., 45
Hu, Jun, 1087
Hu, Ying, 1949
Hyldtoft, J., 595, 2161
Hyöthläinen, J.M.I., 419

Ibrahium, A.A., 2587
Ichikawa, M., 429
Ilieva, S., 739
Iliev, V., 969
Imasato, H., 2575
Ishida, H., 319, 855, 1061, 2397
Itoh, S., 125
Iwahishi, M., 1005
Iwaki, M., 125

Jacobsen, C.J.H., 595, 2161
Janni, J., 2171
Jayaraj, S.E., 979
Jayatyagaraju, V., 65
Jean-Louis, A., 643
Jeergal, P.R., 909
Jiang, Yun-Bao, 275
Jie, Nianqin, 185
Joens, J.A., 247
Johnson, A.F., 2057
Juchnovski, I., 1871
Judkins, M., 2117

Kalkoti, G.B., 909
Kanesaka, I., 941
Kauppinen, R.T., 419
Ke, Weizhong, L25
Kemsley, E.K., 371
Keresztury, G., 429
Khlifi, M., 617
Kim, Hidong, 45
Kini, A.M., 947
Kitano, H., 2433
Klapötke, Th.M., 905
Klapötke, T.M., 1075
Klapstein, D., 787
Klockmann, H.-C., 1939
Klots, T.D., 1255, 1273, 1291, 2307
Kneipp, K., 481, 2171
Kobayashi, M., 125
Koenig, J.L., 2397
Koh, Tse Yuen, 253, 2177
Kolehmainen, E.T., 419, 1543
Kollát, E., 1399
Koll, A., 1935
Korzeniewski, C., 499
Kowalchyk, W.K., 145
Koyama, Y., 1949
Kozhevina, L.I., 2517
Kramer, B., 89
Kroth, H.-J., 1075
Kubista, M., L7
Kudelski, A., 573
Kumar, S., 1459
Kunesch, G., 1861
Kurabe, H., 2447
Kurimoto, Y., 1949
Kuzina, L.A., 1935

Laihia, K.P., 419
Lamcharfi, E., 1861
Lapinski, L., 1809
Lappalainen, K.V., 1543
Lasagabaster, A., 929
Lassègues, J.-C., 1323
Laurenti, E., 437
Laur, P.H., 89
Lawson, E.E., 2057
Leblanc, A., 805
Leciejewicz, J., 303
Le Doucen, R., 1239
Lee, L.V., 45
Le Moel, A., 567
Lenaerts, S., 883
Lewis, I.R., 215, 1985, 2237
Liang, Weian, 177
Li, Jun, 519
Li, Zhe, 1739

Linares, R.M., 1691
Lipiński, J., 381
Li, R.H., 2511
Liu, Fanchen, 1903, 2501
Liu, Shaopu, 1497
Liu, Y., 1005
Liu, Zhongfang, 1497
López Navarrete, J.T., 293, 2347
Luc, P., 1171
Ludwig, C., 2019
Lugtenburg, J., 135
Lutz, H.D., 755

Maafi, M., 603
Maccotta, A., 1959
Machwe, M.K., 1459
Madhukar, K., 65
Maeda, Y., 2433
Maes, G., 883
Maillard, P.A., 1105
Mandelatz, K.W., 89
Manna, B.Kr., 1051
Manfait, M., 1977, 2083
Manogaran, S., 925
Mantsch, H.H., 1399
Mantz, A.W., 2211
Mao, Qinglu, 2459
Marco, C., 2139
Marini, D., 1959
Marsh, D., 111, L1
Martín, C., 1837
Martín, I., 1837
Martin, G.J., 839
Martin, M.L., 839
Martin, P.A., 1117, 1579
Mastryukov, V.S., 215, 2237
Mathews, C.K., 587, 2289
Matousek, P., 2491
Mattioda, A.L., 2545
Maurya, B.P., 661, 1317
McKean, D.C., 215, 685, 2237
McPhail, A.L., 215
McVey, I.F., 2385
Meng, J.X., 2511
Merlin, J.C., 913
Meyer, C., 1861
Meyer, M., 1565
Miller, J.R., 237
Mills, I.M., 769
Mimuro, M., 125
Mincu, I., 349
Mirti, P., 437
Mishra, P.C., 831
Mishra, S.C., 1459
Misra, T.N., 2539
Mitra, S., 363
Mizoguchi, T., 1949
Mlinarić-Majerski, K., 1643
Mohan, S., 735
Mokhlisse, R., 101
Mokhtar-Mohamed, Mohamed, 1, 1525
Molina, M., 929
Molinié, P., 805
Moore, J., 2039
Moreira, W.C., 2325
Moret-Bailly, J., 1231
Morozov, A.I., 1725
Morris, M.D., 145
Mortensen, A., 1345
Mukherjee, S., 363
Murphy, W.F., 215, 2237
Murty, V.S., 731
Murugan, R., 735

Nagaraja Naidu, Y., 2531
Nägele, T., 1565
Nandy, S.K., 2539
Narasimhulu, K.V., 2531
Natkaniec, I., 303
Nau, W.M., 787
Navati, M.S., 909
Nayar, V.U., 429, 1509
Nemes-Vetéssy, Zs., 799
Netto-Ferreira, J.C., 1385
Nicol, L., 839
Nielsen, O.F., 595, 1345, 2161
Nijegorodov, N.I., 2335
Nishio, M., 617
Nour, E.M., 471
Nowak, M.J., 1809
Nozawa, T., 125
Nxumalo, L.M., 1847
Nygren, J., L7
Nyquist, R.A., 475

Oda, K., 941
Ohwada, K., 309
Olivato, P.R., 1479
Osborne, A.G., 237, 2525
Ovsiankina, E., 2465
Ozaki, Y., 1005

Padmavathi, V., 2531
Paez, J.A., 1801
Paillous, P., 617
Palm, K., 1635
Pal, M.K., 489
Panigrahi, B.S., 2289
Panunzio, M., 563
Paoli Monteiro, V.R., 1517
Pardo, A., 1879
Párkányi, C., 603
Parker, A.W., 2491
Parker, S.F., 2067
Parkin, J.E., 961, 1469, 2267, 2273
Parthasarathy, V., 71
Parthiban, S., 2453
Pawlukojc, A., 303
Pellow-Jarman, M.V., 2107
Pereiro-García, R., 895
Perova, T.S., 533
Perrin, A., 1217
Petersohn, E., 567
Peter, S., 2289
Peter, St., 755
Petty, C., 2193
Pfister-Guillouzo, G., 1801
Piart-Goypiron, A., 457
Pichot, Y., 1703
Pietri, N., 1891
Pivovarov, V.B., 843
Plateaux, J.J., 1153
Polo, A.M., 1879
Pope, S.J.A., 2011, 2027
Pop, V., 2441
Pourcin, J., 349
Poyato, J.M.L., 1879
Prasada Rao, T.A., 2473
Prezhdo, O., 2465
Prezhdo, V., 2465
Prokopenko, E.B., 2517
Prusinowska, D., 1809
Pulham, C.R., 769
Punnoose, A., 661, 1317

Quadri, S.M., 1355
Qureshi, P.M., 733

Raap, J., 135
Raghunandan, B.N., 2453
Ramakrishnan, V., 979
Ramírez, F.J., 293, 2347
Ramos, M.N., 821
Rao, J.L., 2531
Ratajczak, H., 197
Ratheesh, R., 429, 1509
Raulin, F., 617
Redondo, M.I., 341
Remizov, A.B., 1725, 1919
Ren, Xin-Min, 717
Ren, Xuozhen, 185
Reva, I.D., 843
Ribeiro, D.S., 1479
Rittner, R., 1479
Rives, V., 1837
Robert, B., 1861
Roggen, J., 883
Rohatgi-Mukherjee, K.K., 1051
Román, F., 2139
Ross, A.J., 1191
Rossi, A., 11
Russell, N.C., 2091
Rybachenko, V.I., 2517

Sadeek, S.A., 471
Sadun, C., 11
Sahai, P., 727
Saito, H., 2447
Salagram, M., 65
Sala-Pala, J., 805
Salvato, B., 1965
Šaman, D., 1543
Sankaran, K., 587
Santo, M., 1749
Sarkar, S.K., 71
Satoh, K., 125
Scheer, H., 1565
Schmidt, S., 1565
Scholz, G., 2481
Schulz, A., 905
Seaward, M.R.D., 2091
Seguin, L., 1323
Severson, M.W., 499

Shahada, L.A., 471
Sham, Y.Y., 247
Shashidhar, M.A., 909
Shaw, R.A., 1399
Shehata, A.K., 1747
Sheina, G.G., 843
Sheng, Rong Sheng, 1087
Sheng, Zhihao, 1031
Shine, K.P., 1393
Shochat, S., 135
Shukla, M.K., 831
Shurvell, H.F., 1355
Sigalov, A.B., L23
Silber, J.J., 1749
Sillence, J.M., 1703
Singh, B., 727
Singh, K.M., 269
Singh, R.A., 269
Singh, R.J., 661, 1317
Sitkowski, J., 839
Sjoback, R., L7
Slarke, D., 2091
Sobhanadri, J., 2473
Sobrinho, E.G., 287
Sockalingum, G.D., 1977, 2083
Sokolov, N.D., 2379
Sokolovskaja, N.V., 1935
Soria, D.B., 677
Spojakina, A., 1837
Starcke, C., 685
Steel, C.J., 1703
Stefaniak, L., 839
Steinfeld, J.I., 2171
Stepanian, S.G., 843
Stephens, S.M., 1413
Stoeva, S., 1965
Stolov, A.A., 1725, 1919
Stoń, M., 1549
Streck, R., 475
Stuart, B.H., 2133
Subramanian, S., 2199
Sumathi, R., 2453
Sünnetçioglu, M.M., 1389
Suppan, P., 1043
Su, Qingde, 2459
Sun, Xiaolin, 1739
Suresh, G., 429, 1509
Suzuki, E., 779, 2447
Suzuki, M., 1005
Suzzi-Valli, G., 563
Swinbourne, F.J., 1703, 1715
Szekeres, M., 799

Tabak, M., 2575
Tait, J.K.F., 2101
Takei, T., 729
Tamiatti, K., 1703
Tarakeshwar, P., 925
Tavladorakis, K., 961, 1469, 2267, 2273
Tedder, D.W., 2301
Teleb, S.M., 471
Téllez, S.C., 395
Temperini, M.L.A., 1517
Thakur, S.N., 269
Thiel, W., 685
Thomas, P.S., 2133
Timney, J.A., 33
Titov, E.V., 2517
Toner, W.T., 2491
Topach, A., 633
Towrie, M., 2491
Tsukahara, N., 729
Tungol, N.W., 1985

Umar, M., 661
Uzoukwu, B.A., 1081

van der Maas, J.H., 2147
van Leeuwen, S., 135
van Liemt, W.B.S., 135
Vankó, Gy, 799
von Nagy-Felsobuki, E.I., 1827
Valensin, G., 1959
Valentin, A., 1127
Van-Than, Nguyen, 643
Varetti, E.L., 669
Velasco-García, N., 895
Velcheva, E., 1871
Verberckmoes, F., 153
Vergès, J., 1191
Verlaque, P., 1891
Vértes, A., 799
Vieira Ferreira, L.F., 1385
Vijgenboom, E., 135
Vij, J.K., 533
Viswanathan, K.S., 587, 2289
Voelter, W., 1965
Vogel-Weill, C., 2357
Vrielynck, L., 913

Wachtveitl, J., 1565
Wallet, J.C., 913
Wang, Feng, 1827
Wang, H.H., 947
Wang, Jianfang, 1683
Wang, Naixing, 177, 185
Wang, Xiuyan, 2501
Wang, Xue-Mei, 333
Wang, Y., 2171
Wang, Yang, 481
Wang, Yingjie, 177
Wang, Yujin, 2501
Wang, Zheng-Yu, 125
Wan, Jian, 1665
Warmsley, J.F., 237, 2525
Watari, F., 779, 2447
Wazeer, M.I.M., 2279
Webb, G.A., 839
Westberg, N., 1017, 1501
West, Y.D., 2011, 2027
Widayati, S., 1413
Williams, A.D., 1413
Williams, J.M., 947
Williams, K.P.J., 549
Winder, S.L., 1753
Wolfs, I., 1601
Woike, Th., 447
Wu, Guozhen, 709
Wu, Jianzhong, L25

Xia, Shuping, 519
Xie, Jian-Wei, 1909
Xin, Howen, 1903, 2501
Xu, Chungi, 2501
Xu, Jin-Gou, 1909
Xu, Zhi San, 1087
Xue, Gi, 1031

Yamaguchi, H., 729
Yan, Sheng-Gang, 2421
Yang, Jinghe, 177, 185
Yang, Y.S., 2511
Yarwood, J., 2101
Ystenes, B.K., 2481
Ystenes, M., 699, 1017, 1501, 2481

Zakharieva, O., 447
Zamama, M., 101
Zarantonello, P., 563
Zeng, Yun'e, 1087
Zhang, Ai-Li, 2421
Zhan, Chang-Guo, 1665
Zhang, Hongguang, 1903, 2501
Zhao, Guiwen, 2459
Zhou, D.J., 2511
Zhou, J.Y., 2511
Zhou, Jie, 177
Zhou, Keyan, 2421
Ziegler, W., 1763
Zimmerman, D.A., 2397
Zin, Min, 1739
Zine, H., 457
Zinth, W., 1565
Zou, Huabin, 185
Zuo, Jian, 2501

SPECTROCHIMICA ACTA

PART A: MOLECULAR AND BIOMOLECULAR SPECTROSCOPY

NOTES FOR CONTRIBUTORS

General

The journal publishes *Letters*, full length *Papers*, *Review Articles* and *Notes*. All contributions should have clear scientific value and report new data, procedures, equipment, or new theoretical considerations, as noted in the Aims and Scope for either "Molecular Spectroscopy" or "Biomolecular Spectroscopy".

Letters are meant for publication of important new results in concise form. *Letters* should not exceed the equivalent of 5000 words including figures and tables. Special attention will be given to ensure rapid publication of contributions accepted as *Letters*.

Papers should be complete and authoritative accounts of work which have special significance, general interest and which are presented clearly and concisely.

Review Articles are commissioned by the Editors on the advice of the Editorial Advisory Board. Authors wishing to submit a review article should contact an Editor or a member of the Board.

Short Notes are short descriptions of work of sufficient interest to justify publication but describing basically well established methodology and/or theory and therefore only available in full through the Deposited Documents scheme. These *Notes* should not exceed the equivalent of 3000 words including figures and tables.

The submission of a contribution for publication in *Spectrochimica Acta Part A* is held to imply that it has not previously been published in any language, that it is not under consideration for publication elsewhere, and that if accepted for publication it will not be published elsewhere without the written approval of the Editors and consent of the Publisher.

Submission of Contributors

Authors should submit their contribution to the appropriate section (Molecular Spectroscopy or Biomolecular Spectroscopy) as follows:

Molecular Spectroscopy

Typescripts should be submitted to one of the Editors: Professor Sidney Kettle or Professor Jeffrey Steinfeld.

Professor Sidney Kettle, School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, U.K.
Fax: +44 1603 507747

Professor Jeffrey Steinfeld, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.
Fax: +1 617 253 7030

Contributions may be written in English, French or German. For all papers an abstract in English must be provided.

Biomolecular Spectroscopy

Typescripts should be submitted to one of the Editors: Professor Arnold Hoff or Professor James Norris, or directly to an expert member of the Editorial Advisory Board for Biomolecular Spectroscopy. Final responsibility for acceptance or rejection always rests with the Editors.

Professor Arnold J. Hoff, Huygens Laboratory, Leiden University, Niels Bohrweg 2, PO Box 9504, 2300 RA Leiden, The Netherlands
Fax: +31 71 275955/5700

Professor James R. Norris, Department of Chemistry, University of Chicago, 5735 S. Ellis Avenue, Chicago, IL 60637, U.S.A.
Fax: +1 312 702 2879

The full addresses of Editorial Advisory Board members are given in the first issue of each volume of the journal.

All contributions must be written in English.

Typescripts may be submitted by fax but should be backed up by submission using normal mail. All authors are requested to include a note of their fax number and/or e-mail address when submitting their typescript.

Format of Contributions

All contributions should be submitted in triplicate. They should be typed on one side of the page only, and the text should be double spaced with wide margins.

Authors should also submit a copy of any paper included in the references which is not yet published, e.g. "in press" or "submitted for publication". To minimize postal charges, submitted materials is not in general returned to authors. Original drawings and photographs can be returned to an author if requested; otherwise these are discarded one month after publication.

In preparing their typescript authors are encouraged to familiarize themselves with, and to follow, the format of articles published in current issues of the journal.

Figures, including Photographs

The original line drawings or photographs for figures should be supplied with one of the copies of the typescript. Each figure should be clearly marked on the back with the names of the authors and the figure number.

Captions for figures should be typed on a separate sheet.

Line drawings should always be carefully prepared at about twice the final size, on plain white drawing paper, and suitable for direct reproduction. Laser printer output at 300 dots per inch for a two-to-one reduction on good quality paper is acceptable. Authors should take particular care to ensure that lettering on a figure will remain clearly legible after reduction.

Photographs should be enlarged sufficiently to permit clear reproduction. If words or numbers appear in photographs two copies are required, one with the words or numbers clearly overprinted and the other without inscription.

Tables

Each *Table* should be supplied on a separate sheet and should include a caption.

Tables should be constructed as to be intelligible without reference to the text, every table and column being provided with a heading. Units of measurement must always be clearly indicated. Unless it is essential to the argument, tables should not list the results of individual experiments, but should summarize results by an accepted method of expression (e.g. standard deviation). The same information should not be produced in both tables and figures.

Units

SI units are required.

Nomenclature

All nomenclature should conform as closely as possible to the rules established by IUPAC and IUPAP, as summarized in the following publications: N. Sheppard, H.A. Willis and J.C. Rigg, Spectrochimica Acta Part A, 43 (1987) 1; E.R. Cohen and P. Giacomo, Physica, 146A (1987) 1–68; I. Mills et al., Quantities, Units and Symbols in Physical Chemistry, Blackwell, Oxford (1988).

References

References should be indicated in the text by consecutive numbers in square brackets; the full references should be listed at the end of the paper in the following form:

[1] C.J. Pedersen, J. Am. Chem. Soc., 89 (1967) 7017.
[2] J.D. Lamb, R.M. Izatt, J.J. Christensen and D.J. Eatough, in Coordination Chemistry of Macrocyclic Compounds, G.A. Melson (Ed.), Chap. 1, Plenum Press, New York, 1979.
[3] R.M. Izatt, J.S. Bradshaw, S.A. Nielsen, J.D. Lamb, J.J. Christensen and D. Sen, Chem. Rev., 85 (1985) 271.
[4] R.D. Amos, Advances in Chemical Physics, I. Prigogine and S.A. Rice (Eds.), Vol. 67, p. 99. Wiley, New York, 1987.

Journal-name abbreviations should follow those adopted by The Chemical Abstracts Service (Bibliographic Guide for Editors and Authors, The American Chemical Society, Washington, DC, 1974).

Proofs, Reprints and Copyright

Proofs: Where multiple authors are concerned it is important to indicate, when submitting a contribution, the author to whom correspondence and proofs should be sent. Only essential corrections should be made at proof stage. Alterations to the text, other than printer's errors, may be charged to the author.
The Publisher reserves the right to publish a contribution without waiting for corrected proofs to be returned by the author, if waiting would cause undue delay.
Reprints: No page charges are assessed and 25 free reprints will be provided to the principal author. Authors should indicate the number of additional paid reprints required when returning their proofs.
Copyright: Authors are requested to read the note on copyright published on the verso of the title page of each issue. Publication of a contribution may have to be delayed until a signed transfer of copyright agreement has been received by mail. Authors are recommended to send the agreement at the same time as the proofs are returned.

Deposited Documents

From time to time, the journal receives typescripts which contain extensive tabular or graphical data. Though such data may be of archival interest, and should be available to workers in the field, it is often impractical to publish such material in its entirety. For this reason, the journal has entered into a supplementary data deposition scheme with the British Library Document Supply Centre, details of which have been given in the last page of *Spectrochim. Acta Part A*, 43 No. 6 (June 1987). Authors are encouraged to avail themselves of this service when appropriate. Persons wishing to obtain copies of deposited material should write, citing the accession number, directly to Service Enquiries, British Library Lending Library, Document Supply Centre, Boston Spa, Wetherby, West Yorkshire LS23 7BQ, U.K. Requesters must quote the relevant SUP number (e.g. SUP 12345). Supplementary Publications are made available on a pro forma invoice basis.